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# MEMORANDUM

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| **To:** | Dr. Robert Law and Willard Potter, de maximis, inc. | **Date:** | December 8, 2016 |
| **From:** | Wen Ku, Peter Oates, Peter Israelsson, and John Connolly, Anchor QEA, LLC | **Project:** | 120980-02.05 |
| **Re:** | Proposed COPCs to be Calibrated in the Lower Passaic River/Newark Bay Contaminant Fate and Transport Model | | |

During the modeling meeting on June 28, 2016, representatives of the U.S. Environmental Protection Agency (USEPA) Region 2 and the Cooperating Parties Group (CPG) discussed the chemicals of potential concern (COPCs) to be modeled in the Lower Passaic River/Newark Bay (LPR/NB) contaminant fate and transport (CFT) model. The CPG expressed concern about the level of effort and value of modeling all 29 COPCs requested by Region 2 in its comment to the 17-mile Lower Passaic River Study Area (LPRSA) Remedial Investigation (RI) Report (USEPA 2016a; Comment 372). The CPG argued that a number of the listed chemicals were not likely to influence remedial decision-making and including them would not materially strengthen assessments of the robustness of process parameterizations in the model. The CPG advocated focusing on COPCs likely to influence remedial decision-making and additional chemicals that fill gaps in the range of characteristics needed to assess process parameterization robustness. Region 2 agreed in principle and asked the CPG to propose a subset of COPCs to be modeled that takes account of COPC contributions to risk, considering the 48 COPCs simulated by Region 2 in the Focused Feasibility Study (FFS)/Record of Decision (ROD) model (LBG et al. 2014; USEPA 2016b). Region 2 also agreed that the CPG can focus its calibration efforts on a subset of the selected COPCs and treat the remainder as secondary calibration support (per Region 2's approach in the FFS [LBG et al. 2014]). In order to reduce the effort on COPC mapping, Region 2 further agreed that the conditional simulation-based mapping need only to be performed for COPCs of main focus in the remediation benefit evaluation; Thiessen polygon-based mapping may be used for the remainder.

This memorandum describes the method used to select the COPCs that the CPG proposes to model, which incorporates Region 2's feedback during the September 20, 2016 modeling meeting and in an email communication on October 4, 2016. The goal of this selection process is to minimize the number of COPCs required for simulation while still meeting the needs of the 17-mile LPRSA RI and addressing the concerns raised by Region 2.

## COPC Selection Method

The proposed COPCs were selected from the 48 FFS/ROD model COPCs using the four criteria below:

1. **Risk:** Given that the objective of the modeling is to predict reductions in risk achieved by remedial alternatives, risk is the primary selection criterion. COPCs are chosen for calibration if the baseline human health carcinogenic risk is greater than or equal to $10^{-5}$ and/or the non-carcinogenic hazard quotient (HQ) is greater than or equal to 1. This threshold of carcinogenic risk is within the risk range of $10^{-4}$ to $10^{-6}$ that Region 2 specified as the remediation goal in the ROD for the lower 8.3 miles of the LPR (USEPA 2016b). The threshold of the non-carcinogenic HQ of 1 is also consistent with the ROD. It is assumed that COPCs with risks below these thresholds would not factor strongly into remedial decision-making, under the expectation that the risk they pose would be reduced as a result of the active remediation and/or natural recovery. Thus, those COPCs are not selected for inclusion in the CFT model unless supported by other criteria. Furthermore, COPCs identified as ecological risk drivers are also selected.

2. **Octanol-water partition coefficient (Kow):** For the hydrophobic organic compounds of primary focus in the LPR/NB model, Kow values are used to characterize sorptive properties in the selection methodology. Sorption affects the extent to which COPC fate is controlled by processes associated with dissolved and sorbed chemical. Region 2 commented that the Kow values for 2,3,7,8-tetrachlorodibenzo-p-dioxin (TCDD) and tetrachlorobiphenyl (tetra-CB) (i.e., the COPCs calibrated in the draft 17-mile LPRSA RI [Anchor QEA et al. 2015]) are at the low end of the range of values for the 29 polychlorinated dibenzo-p-dioxin (PCDD), polychlorinated dibenzofuran (PCDF), and polychlorinated biphenyl (PCB) congeners that are targeted for

calibration in Region 2's 2006 *Final Modeling Work Plan* (HQI 2006) and thus do not fully explore the model's transport of sorbed chemical. To address Region 2's concern, if the Kow values of the COPCs selected using the risk criteria do not cover a sufficiently broad range of Kow (using values from the FFS/ROD model [LBG et al. 2014]), additional COPCs are chosen to fill out the range. This criterion results in adding chemicals of lower risk, but higher Kow (and higher organic carbon-water partition coefficient [Koc[1]]).

3. **Frequency of detection:** COPCs with many non-detect samples in the water column and/or sediments are poor candidates for calibration. The frequency of detection is used to choose among COPCs with lower risk but high Kow being considered to fill out the Kow range. The frequency of detection is also used to determine whether a selected COPC will be considered primary or secondary in the calibration process. Although all COPCs will be subject to the same model-data comparison metrics, more weight will be given to the model-data agreement of the primary calibration COPCs when setting parameter values that are not COPC-specific (e.g., sediment mixing). At least 80% of detect samples from the small-volume chemical water column monitoring (sv-CWCM) are needed for a primary calibration COPC. Similarly, at least 80% detect samples in the sediments will be required for a given primary calibration COPC so that reasonable sediment initial conditions can be developed and a reliable long-term trajectory can be derived for the sediment calibration. The availability of high-volume chemical water column monitoring (hv-CWCM) measurements above the detection limit is also considered in selecting additional COPCs, as these data are used to characterize site-specific sorption within the partitioning framework proposed by the CPG at the June 28, 2016 meeting with Region 2.

4. **Correlation among selected COPC congeners:** Correlations among selected COPCs that are congeners of the same chemical group (e.g., PCBs, dioxins, furans) were examined using linear regressions of surface sediment and water column

[1] Koc was referenced in Region 2's edits to action items in the draft summary of the June 28, 2016 meeting; the result of the COPC selection presented below would not be altered if based on a Koc range rather than a Kow range.

concentrations. Strong correlation of sediment concentrations suggests a corresponding similarity in the pattern of integrated contaminant fluxes to/from the surface sediments over the long term (i.e., reflecting a balance of initial conditions, boundary conditions, and transport mechanisms within the LPR). Likewise, strong correlation in the sv-CWCM data suggests that present-day fluxes to the water column are also similar in pattern. Only one congener per set of strongly correlated congeners is selected for simulation in the CFT model; concentrations of the remaining congeners could be predicted from the modeled congener using data regressions if needed for risk assessment, but would not factor into the calibration of the model.

## COPC Selection Results

Table 1 summarizes the CPG risk estimates, chemical properties, and detection frequencies in the sediment and water column data for each of the 48 COPCs included in Region 2's CFT model for the FFS/ROD, among which are the 29 that were the subject of the aforementioned Region 2 comment. The values of Kow and other chemical properties listed in Table 1 are those used in the FFS/ROD model (Table 3-7; LBG et al. 2014). Three-phase apparent[2] Koc values were calculated using hv-CWCM data and included in Table 1 at Region 2's request, reported as an average for samples within the LPR and LPR/NB (considering only those with detected dissolved chemical concentrations). The risk estimates are based on CPG's baseline human health risk assessment (BHHRA; AECOM 2015) and baseline ecological risk assessment (BERA; Windward 2016). To evaluate human health risk, reasonable maximum exposure (RME) risks through fish consumption for current and future anglers are used, on an individual congener basis. To evaluate ecological risk, HQs for individual COPCs are not provided because multiple receptors are evaluated in the BERA. Rather, COPCs are flagged as ecological risk drivers in Table 1 if the BERA identified significant risk for one or more receptors. The frequencies of detection are reported for the sv-CWCM and hv-CWCM datasets across all LPR/NB stations and for LPR stations alone,

[2] The values reported in Table 1 are regarded as apparent Koc values because they reflect an unknown state of equilibrium between dissolved and sorbed contaminant in the water column. As such, they are not proposed for direct incorporation into the model parameterization. The hv-CWCM data will instead be used within the CPG's proposed water column partitioning framework, with parameterization details to be provided to Region 2 under separate cover as follow-up to the September 20 meeting.

and for the surface (top 6 inches) sediment data in the "1995" and "2010" contaminant mapping datasets.[3]

Nine COPCs are proposed for modeling on the basis of the above-selection methodology. These COPCs are highlighted in Table 1, which also shows the proposed level of calibration and type of mapping to be used in simulations. The basis of each selection is briefly summarized below:

- Primary COPCs for calibration:
  - 2,3,7,8-TCDD: Human health cancer risk > $10^{-4}$ and HQ > 10; also an identified ecological risk driver
  - Tetra-CB[4]: To estimate total PCBs (via the data-based regressions shown in Figure 1 and Table 2), which has human health cancer risk > $10^{-4}$ and HQ > 10, and is an identified ecological risk driver.
  - 1,2,3,4,6,7,8-HpCDF: High log Kow (8.67) [and log Koc (9.37)] and high frequency of detection. This congener is also one of the five major congeners found in the Phase 1 removal footprint near Lister Avenue.
  - PCB-167: Intermediate log Kow (7.27) [and log Koc (8.44)] and high frequency of detection.
- Secondary COPCs for calibration:
  - PCB-126: Human health cancer risk > $10^{-4}$ and HQ > 10.
  - 1,2,3,7,8-PeCDD: Human health cancer risk between $10^{-5}$ and $10^{-4}$ and HQ between 1 and 10.
  - 2,3,4,7,8-PeCDF: Human health cancer risk between $10^{-5}$ and $10^{-4}$ and HQ between 1 and 10.
  - Mercury: As a surrogate for methyl mercury[5], which has human health HQ between 1 and 10. Both mercury and methyl mercury are identified as ecological risk drivers.

[3] The 1995 and 2010 datasets used for contaminant mapping contain samples collected from 1995 to 1999, and 2005 to 2013, respectively.
[4] It was concluded from regression analysis that only a marginal improvement will likely be achieved in predicting total PCBs by modeling additional PCB homologs, such as tri-CB and penta-CB.
[5] Modeling methyl mercury as total mercury with an average conversion factor avoids uncertainty in methyl mercury production/destruction dynamics.

- Total DDx: Identified as an ecological risk driver. It is proposed to simulate total DDx as a single compound rather than as six individual congeners; the Kow and Koc for all six congeners are within an order of magnitude (Table 1) and simulating them as a group is analogous to simulating a PCB homolog.

Although PCB-105 and PCB-118 meet the applied risk criteria, they were not selected because of their strong correlation with PCB-167 (see Figure 2; $R^2$ values are 0.94 or higher). Concentrations of these two congeners will not be simulated but can be computed if needed based on the calibrated PCB-167 results using the equations listed in Table 2.

Although the BERA identified PCDD/PCDF, PCB, and total Toxic Equivalency Quotient (TEQ) as ecological risk drivers, for tractability the proposed list was not expanded to include all contributing congeners (TEQ is based on 17 dioxin and furan congeners and/or 12 PCB congeners). Rather, it is proposed that PCDD/PCDF TEQ can be computed if needed from model predictions of the four PCDD/PCDF congeners selected above (i.e., 2,3,7,8-TCDD, 1,2,3,7,8-PeCDD, 2,3,4,7,8-PeCDF, and 1,2,3,4,6,7,8-HpCDF), using the relationships shown in Figure 3. Similarly, PCB TEQ can be computed from the two PCB congeners selected for simulation (i.e., PCB-126 and PCB-167) plus PCB-105 and PCB-118 (calculated from PCB-167 predictions as described above). It follows that total TEQ can be computed as a function of the six proposed model PCDD/PCDF and PCB congeners, plus PCB-105 and PCB-118. The equations to compute PCDD/PCDF TEQ, PCB TEQ and total TEQ are presented in Table 2, based on the regressions shown in Figure 3.[6] It is noted that a potential adjustment to the application of regressions is to combine the bed and water column data to derive a single regression equation for both media, which could be pursued if preferred by Region 2.

It is assumed that delineation of active remediation areas for the purpose of constructing Feasibility Study alternatives will be accomplished using the spatial distributions of sediment 2,3,7,8-TCDD and total PCBs, as predicted from tetra-CB concentrations. Consequently, it is proposed that conditional simulation-based mapping be performed only for these two COPCs

[6] Non-detect congeners were set to zero when computing TEQ. TEQ was not computed if all the totaling congeners were not analyzed or if all congeners were non-detects. A few high TEQ sample values were excluded in the water column regressions: 11A-CE04-TTR1-A and 12F-CE04-TTR1-B for PCDD/PCDF TEQ and total TEQ, as well as 12G-CE02-T102-B for PCB TEQ (as noted in Figure 3).

and that Thiessen polygon-based mapping be performed for the remaining seven COPCs that were selected.

## References

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HQI (HydroQual Inc.), 2006. *Final Modeling Work Plan.* Lower Passaic River Restoration Project. Mahwah, New Jersey.

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# TABLES

**Table 1**

**Chemical Properties, Estimated Risk, and Data Detection Frequency for COPCs Simulated in Region 2's FFS Contaminant Fate and Transport Model, and Summary of CPG's Proposed Selection for Simulation in the RI/FS Model**

| Name | Estimated Risk | | | Chemical Properties[3] | | | | | | | | | | % Detection in hv-CWCM Dataset[5] | | % Detection in sv-CWCM Dataset[6] | | % Detection in Surface Sediments[7] | | Proposed Level of Calibration in RI/FS Model | Proposed Type of Mapping in RI/FS Model | Reasons to Include in or Exclude from Proposed Selection for RI/FS Model |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | HH Cancer Risk[1] | HH Non-Cancer Hazard Quotient (HQ)[1] | Ecological Risk Driver[2] | Molecular Weight (g/mole) | Log Kow (L/Kg) | Log Koc (L/Kg) | $A_{DOC}$ | $\Delta H_{OW}$ (KJ/mole) | $K^{salt}$ | Henry's Constant (Pa $m^3$/mole) | $\Delta H_{AW}$ (KJ/mole) | hv-CWCM Log Koc – LPR/NB[4] (L/kg) | hv-CWCM Log Koc – LPR Only[4] (L/kg) | LPR/NB | LPR Only | LPR/NB | LPR Only | 1995 Dataset[8] | 2010 Dataset[9] | | | |
| 2378-TCDD | 1.89E-03 | 99 | Yes | 322.0 | 6.65 | 6.81 | 0.08 | 0.0 | 0.35 | 1.42 | 0 | 7.79 | 7.89 | 79% | 81% | 71% | 87% | 99% | 99% | Primary | CS | HH risk; ecological risk driver |
| 12378-PeCDD | 2.76E-05 | 1.4 | | 356.4 | 7.37 | 7.18 | 0.08 | 0.0 | 0.35 | 1.38 | 0 | 6.98 | ND | 31% | 35% | 6.0% | 7.5% | 81% | 94% | Secondary | Thiessen | HH risk |
| 123478-HxCDD | 1.19E-06 | < 0.10 | | 390.9 | 8.12 | 8.20 | 0.08 | 0.0 | 0.35 | 1.28 | 0 | ND | ND | 33% | 35% | 7.4% | 9.8% | 92% | 95% | | | Relatively low HH risk; frequently below detection limit in water column |
| 123678-HxCDD | 4.03E-06 | .21 | | 390.9 | 8.09 | 8.53 | 0.08 | 0.0 | 0.35 | 1.35 | 0 | 9.04 | 9.04 | 40% | 46% | 25% | 37% | 98% | 98% | | | Relatively low HH risk; frequently below detection limit in water column |
| 123789-HxCDD | 1.28E-06 | < 0.10 | | 390.9 | 8.10 | 8.59 | 0.08 | 0.0 | 0.35 | 1.26 | 0 | 8.49 | 8.90 | 44% | 58% | 28% | 33% | 95% | 97% | | | Relatively low HH risk; frequently below detection limit in water column |
| 1234678-HpCDD | < $10^{-6}$ | < 0.10 | | 425.3 | 8.82 | 9.89 | 0.08 | 0.0 | 0.35 | 1.23 | 0 | 10.48 | 10.60 | 65% | 77% | 80% | 87% | 99% | 100% | | | Low HH risk |
| OCDD | < $10^{-6}$ | < 0.10 | | 459.8 | 9.57 | 10.90 | 0.08 | 0.0 | 0.35 | 1.21 | 0 | 11.43 | 11.43 | 62% | 81% | 91% | 94% | 99% | 99% | | | Low HH risk; strong boundary influence |
| 2378-TCDF | 3.03E-06 | 0.16 | Yes (as PCDD/PCDF TEQ and total TEQ) | 306.0 | 6.54 | 6.87 | 0.08 | 0.0 | 0.35 | 2.49 | 0 | 7.71 | 7.81 | 81% | 77% | 31% | 40% | 99% | 97% | | | Relatively low HH risk; frequently below detection limit in water column |
| 12378-PeCDF | < $10^{-6}$ | < 0.10 | | 340.4 | 7.25 | 7.28 | 0.08 | 0.0 | 0.35 | 2.18 | 0 | ND | ND | 38% | 42% | 13% | 18% | 97% | 96% | | | Low HH risk |
| 23478-PeCDF | 2.08E-05 | 1.1 | | 340.4 | 7.23 | 7.38 | 0.08 | 0.0 | 0.35 | 2.36 | 0 | 8.31 | 8.31 | 56% | 65% | 29% | 41% | 98% | 98% | Secondary | Thiessen | HH Risk |
| 123478-HxCDF | 6.23E-06 | 0.33 | | 374.9 | 7.96 | 7.97 | 0.08 | 0.0 | 0.35 | 2.01 | 0 | 8.05 | 8.25 | 58% | 73% | 66% | 77% | 99% | 99% | | | Relatively low HH risk; Kow range covered by other chemicals with higher detection frequency |
| 123678-HxCDF | 2.08E-06 | 0.11 | | 374.9 | 7.95 | 8.16 | 0.08 | 0.0 | 0.35 | 2.06 | 0 | 9.39 | 9.39 | 42% | 46% | 36% | 48% | 99% | 98% | | | Relatively low HH risk; frequently below detection limit in water column |
| 123789-HxCDF | < $10^{-6}$ | < 0.10 | | 374.9 | 7.95 | 6.97 | 0.08 | 0.0 | 0.35 | 1.98 | 0 | 7.67 | 7.69 | 1.9% | 0% | 0.9% | 1.1% | 90% | 37% | | | Low HH risk |
| 234678-HxCDF | 1.08E-06 | < 0.10 | | 374.9 | 7.96 | 8.04 | 0.08 | 0.0 | 0.35 | 1.93 | 0 | 9.41 | 9.41 | 48% | 54% | 30% | 44% | 99% | 98% | | | Relatively low HH risk; frequently below detection limit in water column |

**Table 1**

**Chemical Properties, Estimated Risk, and Data Detection Frequency for COPCs Simulated in Region 2's FFS Contaminant Fate and Transport Model, and Summary of CPG's Proposed Selection for Simulation in the RI/FS Model**

| Name | Estimated Risk | | | Chemical Properties[3] | | | | | | | | | | % Detection in hv-CWCM Dataset[5] | | % Detection in sv-CWCM Dataset[6] | | % Detection in Surface Sediments[7] | | Proposed Level of Calibration in RI/FS Model | Proposed Type of Mapping in RI/FS Model | Reasons to Include in or Exclude from Proposed Selection for RI/FS Model |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | HH Cancer Risk[1] | HH Non-Cancer Hazard Quotient (HQ)[1] | Ecological Risk Driver[2] | Molecular Weight (g/mole) | Log Kow (L/Kg) | Log Koc (L/Kg) | $A_{DOC}$ | $\Delta H_{OW}$ (KJ/mole) | $K^{salt}$ | Henry's Constant (Pa $m^3$/mole) | $\Delta H_{AW}$ (KJ/mole) | hv-CWCM Log Koc – LPR/NB[4] (L/kg) | hv-CWCM Log Koc – LPR Only[4] (L/kg) | LPR/NB | LPR Only | LPR/NB | LPR Only | 1995 Dataset[8] | 2010 Dataset[9] | | | |
| 1234678-HpCDF | < $10^{-6}$ | < 0.10 | | 409.3 | 8.67 | 9.37 | 0.08 | 0.0 | 0.35 | 1.75 | 0 | 10.92 | 10.72 | 63% | 69% | 84% | 87% | 99% | 100% | Primary | Thiessen | Low HH risk but with high Kow and high frequency of detected samples; one of the five major congeners in the Lister Avenue Phase 1 removal fingerprint |
| 1234789-HpCDF | < $10^{-6}$ | < 0.10 | | 409.3 | 8.67 | 8.74 | 0.08 | 0.0 | 0.35 | 1.75 | 0 | ND | ND | 33% | 35% | 16% | 23% | 98% | 95% | | | Low HH risk |
| OCDF | < $10^{-6}$ | < 0.10 | | 443.8 | 9.37 | 10.30 | 0.08 | 0.0 | 0.35 | 1.6 | 0 | 11.20 | 11.20 | 42% | 46% | 76% | 78% | 99% | 100% | | | Low HH risk |
| Mono-CB | – | – | | 188.7 | 4.63 | 6.39 | 0.08 | -22.9 | 0.35 | 20.4 | 50.7 | 6.33 | 6.15 | 81% | 69% | 83% | 88% | 100% | 99% | | | Not needed for adequate estimate of total PCBs |
| Di-CB | – | – | | 223.1 | 5.00 | 6.04 | 0.08 | -23.5 | 0.35 | 23.8 | 48.7 | 5.94 | 5.81 | 90% | 92% | 100% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Tri-CB | – | – | | 257.5 | 5.60 | 6.20 | 0.08 | -24.2 | 0.35 | 28.1 | 42.5 | 6.02 | 5.93 | 85% | 92% | 100% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Tetra-CB | – | – | | 292.0 | 6.00 | 6.27 | 0.08 | -24.9 | 0.35 | 36 | 27.7 | 6.27 | 6.35 | 88% | 92% | 100% | 100% | 100% | 100% | Primary | CS | To estimate total PCBs |
| Penta-CB | – | – | | 326.4 | 6.45 | 6.62 | 0.08 | -25.7 | 0.35 | 45.2 | 33.5 | 6.86 | 6.99 | 96% | 100% | 100% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Hexa-CB | – | – | Yes (as PCB TEQ and total TEQ) | 360.9 | 6.85 | 7.15 | 0.08 | -26.8 | 0.35 | 57.5 | 67.3 | 7.46 | 7.62 | 94% | 100% | 100% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Hepta-CB | – | – | | 395.3 | 7.22 | 7.75 | 0.08 | -27.6 | 0.35 | 58.1 | 111 | 8.17 | 8.11 | 71% | 73% | 99% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Octa-CB | – | – | | 429.8 | 7.63 | 8.21 | 0.08 | -28.4 | 0.35 | 40.8 | 160 | 8.96 | 8.90 | 69% | 65% | 99% | 100% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Nona-CB | – | – | | 464.2 | 7.99 | 8.72 | 0.08 | -29.3 | 0.35 | 63.8 | 154 | 9.72 | 9.91 | 69% | 77% | 98% | 99% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |
| Deca-CB | – | – | | 498.7 | 8.18 | 9.01 | 0.08 | -29.9 | 0.35 | 97.5 | 145 | 10.09 | 10.39 | 65% | 65% | 92% | 91% | 100% | 100% | | | Not needed for adequate estimate of total PCBs |

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| | Estimated Risk | | | Chemical Properties[3] | | | | | | | | | | % Detection in hv-CWCM Dataset[5] | | % Detection in sv-CWCM Dataset[6] | | % Detection in Surface Sediments[7] | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Name | HH Cancer Risk[1] | HH Non-Cancer Hazard Quotient (HQ)[1] | Ecological Risk Driver[2] | Molecular Weight (g/mole) | Log Kow (L/Kg) | Log Koc (L/Kg) | $A_{DOC}$ | Δ $H_{OW}$ (KJ/mole) | $K^{salt}$ | Henry's Constant (Pa $m^3$/mole) | Δ $H_{AW}$ (KJ/mole) | hv-CWCM Log Koc – LPR/NB[4] (L/kg) | hv-CWCM Log Koc – LPR Only[4] (L/kg) | LPR/NB | LPR Only | LPR/NB | LPR Only | 1995 Dataset[8] | 2010 Dataset[9] | Proposed Level of Calibration in RI/FS Model | Proposed Type of Mapping in RI/FS Model | Reasons to Include in or Exclude from Proposed Selection for RI/FS Model |
| PCB-77 | 1.58E-06 | < 0.10 | | 292.0 | 6.36 | 7.46 | 0.08 | -28.2 | 0.35 | 16.7 | 57.5 | 7.20 | 7.13 | 100% | 100% | 99% | 99% | 98% | 99% | | | Relatively low HH risk; Kow range covered by other chemicals |
| PCB-81 | < $10^{-6}$ | < 0.10 | | 292.0 | 6.36 | 6.69 | 0.08 | -28.2 | 0.35 | 25.8 | 57.5 | 6.71 | 6.57 | 44% | 19% | 43% | 52% | 100% | 79% | | | Low HH risk |
| PCB-105 | 1.70E-05 | 0.89 | | 326.4 | 6.65 | 7.64 | 0.08 | -27.9 | 0.35 | 33.9 | 59.5 | 7.30 | 7.37 | 98% | 100% | 99% | 99% | 99% | 100% | | | HH risk, but not selected due to strong correlation with PCB-167 |
| PCB-114 | 1.21E-06 | < 0.10 | | 326.4 | 6.65 | 7.57 | 0.08 | -27.9 | 0.35 | 36.7 | 59.5 | 7.17 | 7.20 | 85% | 77% | 91% | 95% | 95% | 97% | | | Relatively low HH risk; Kow range covered by other chemicals |
| PCB-118 | 4.69E-05 | 2.4 | | 326.4 | 6.74 | 7.65 | 0.08 | -27.9 | 0.35 | 36.3 | 59.5 | 7.29 | 7.39 | 98% | 100% | 99% | 98% | 100% | 100% | | | HH risk, but not selected due to strong correlation with PCB-167 |
| PCB-123 | < $10^{-6}$ | < 0.10 | | 326.4 | 6.74 | 7.34 | 0.08 | -27.9 | 0.35 | 36.7 | 59.5 | 7.22 | 7.28 | 88% | 85% | 91% | 94% | 92% | 97% | | | Low HH risk |
| PCB-126 | 3.03E-04 | 16 | Yes (as PCB TEQ and total TEQ) | 326.4 | 6.89 | 7.42 | 0.08 | -29.8 | 0.35 | 21.3 | 60.5 | 7.39 | ND | 52% | 35% | 45% | 57% | 42% | 90% | Secondary | Thiessen | HH risk |
| PCB-156 | 7.96E-06 | 0.41 | | 360.9 | 7.18 | 8.37 | 0.08 | -29.4 | 0.35 | 37 | 62.4 | 8.18 | 8.13 | 77% | 85% | 93% | 94% | 98% | 98% | | | Relatively low HH risk; Kow range covered by other chemicals |
| PCB-157 | < $10^{-6}$ | < 0.10 | | 360.9 | 7.18 | 8.37 | 0.08 | -29.4 | 0.35 | 37 | 62.4 | 8.18 | 8.13 | 77% | 85% | 93% | 94% | 94% | 98% | | | Low HH risk |
| PCB-167 | 3.23E-06 | 0.17 | | 360.9 | 7.27 | 8.44 | 0.08 | -29.4 | 0.35 | 39.2 | 62.4 | 8.07 | 8.31 | 88% | 88% | 97% | 99% | 97% | 99% | Primary | Thiessen | Relatively low HH risk, but intermediate Kow and high frequency of detected samples |
| PCB-169 | 1.33E-06 | < 0.10 | | 360.9 | 7.42 | 7.35 | 0.08 | -31.3 | 0.35 | 23.4 | 63.4 | 7.13 | 7.10 | 7.7% | 15% | 17% | 27% | 6% | 17% | | | Relatively low HH risk; frequently below detection limit in water column |
| PCB-189 | 1.08E-06 | < 0.10 | | 395.3 | 7.71 | 8.33 | 0.08 | -31.0 | 0.35 | 28.8 | 65.3 | 8.90 | 9.36 | 56% | 58% | 51% | 65% | 89% | 96% | | | Relatively HH low risk; Kow range covered by other chemicals with higher detection frequency |

**Table 1**

**Chemical Properties, Estimated Risk, and Data Detection Frequency for COPCs Simulated in Region 2's FFS Contaminant Fate and Transport Model, and Summary of CPG's Proposed Selection for Simulation in the RI/FS Model**

| | Estimated Risk | | | Chemical Properties[3] | | | | | | | | | | % Detection in hv-CWCM Dataset[5] | | % Detection in sv-CWCM Dataset[6] | | % Detection in Surface Sediments[7] | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Name | HH Cancer Risk[1] | HH Non-Cancer Hazard Quotient (HQ)[1] | Ecological Risk Driver[2] | Molecular Weight (g/mole) | Log Kow (L/Kg) | Log Koc (L/Kg) | $A_{DOC}$ | Δ $H_{OW}$ (KJ/mole) | $K^{salt}$ | Henry's Constant (Pa $m^3$/mole) | Δ $H_{AW}$ (KJ/mole) | hv-CWCM Log Koc – LPR/NB[4] (L/kg) | hv-CWCM Log Koc – LPR Only[4] (L/kg) | LPR/NB | LPR Only | LPR/NB | LPR Only | 1995 Dataset[8] | 2010 Dataset[9] | Proposed Level of Calibration in RI/FS Model | Proposed Type of Mapping in RI/FS Model | Reasons to Include in or Exclude from Proposed Selection for RI/FS Model |
| 2,4'-DDD | < $10^{-6}$ | < 0.10 | Yes (as total DDx) | 320.1 | 6.08 | 6.41 | 0.08 | 0.0 | 0 | 0.85 | 0 | NS | NS | NS | NS | 88% | 95% | 8% | 94% | Secondary | Thiessen | Simulate combined as total DDx, which is an ecological risk driver |
| 2,4'-DDE | < $10^{-6}$ | < 0.10 | | 318.0 | 6.72 | 7.07 | 0.08 | 0.0 | 0 | 4.61 | 0 | NS | NS | NS | NS | 56% | 67% | 8% | 90% | | | |
| 2,4'-DDT | < $10^{-6}$ | < 0.10 | | 354.5 | 6.60 | 6.85 | 0.08 | 0.0 | 0 | 2.86 | 0 | NS | NS | NS | NS | 29% | 45% | 0% | 78% | | | |
| 4,4'-DDD | 2.21E-06 | 0.10 | | 320.1 | 6.18 | 6.42 | 0.08 | 0.0 | 0 | 0.74 | 0 | NS | NS | NS | NS | 93% | 99% | 75% | 90% | | | |
| 4,4'-DDE | 5.38E-06 | 0.17 | | 318.0 | 6.79 | 7.26 | 0.08 | 0.0 | 0 | 4.63 | 0 | NS | NS | NS | NS | 86% | 92% | 80% | 96% | | | |
| 4,4'-DDT | < $10^{-6}$ | < 0.10 | | 354.5 | 6.73 | 7.38 | 0.08 | 0.0 | 0 | 2.36 | 0 | NS | NS | NS | NS | 63% | 74% | 58% | 83% | | | |
| Cadmium | < $10^{-6}$ | < 0.10 | No | 112.4 | – | – | – | 0.0 | 0 | 0.000329 | 0 | NS | NS | NS | NS | 100% | 100% | 96% | 96% | | | Low HH risk; no ecological risk |
| Mercury | < $10^{-6}$ | .17 | Yes | 200.6 | – | – | – | 0.0 | 0 | 729 | 0 | NS | NS | NS | NS | 100% | 100% | 94% | 99% | Secondary | Thiessen | As a surrogate for methyl mercury, for reasons noted below; ecological risk driver |
| Methyl Mercury | – | 2.2 | Yes | 215.6 | – | – | – | 0.0 | 0 | 0.000329 | 0 | NS | NS | NS | NS | 95% | 100% | NS | 99% | | | Non-cancer HH risk; ecological risk driver. Model as total mercury with an average conversion factor, to avoid uncertainty in methyl mercury production/destruction dynamics |

Notes:
The highlighted rows are the proposed chemicals of potential concern (COPCs) to be simulated in the contaminant fate and transport model, with the exception of the DDx congeners which are proposed to be simulated together as total DDx.
Percent detection for polychlorinated biphenyl (PCB) homologs in surface sediments does not include those derived from total PCBs.

CS = conditional simulation
CWCM = chemical water column monitoring
FFS = Focused Feasibility Study
hv = high volume
HH = human health
LPR = Lower Passaic River
– = not available
NB = Newark Bay
ND = No detected dissolved chemical concentrations in LPR or LPR/NB
NS = not sampled
PCB = polychlorinated biphenyl
RI/FS = Remedial Investigation/Feasibility Study
RME = reasonable maximum exposure
sv = small volume
TEQ = toxic equivalency quotient

1. Based on RME fish consumption risks/hazards in the CPG baseline human health risk assessment, provided by AECOM.
2. Based on CPG baseline ecological risk assessment, provided by Windward Environmental.
3. Chemical properties from Table 3-7 of the 2014 USEPA FFS model report (LBG et al. 2014, Appendix BIII), with the exception of the Koc values derived from the hv-CWCM dataset (see footnote 4).
4. Average three-phase "apparent" Koc calculated using hv-CWCM data. Samples with non-detect dissolved chemical concentrations were excluded from the calculation. Non-detect organic carbon data set to ½ MDL.
5. Based on contaminant data from all stations measured in the hv-CWCM program.
6. Excluding data measured upstream of Dundee Dam and in the tributaries, the Hackensack River, and the Kills.
7. Surface sediments denotes the top 6 inches of sediment.
8. The "1995" contaminant mapping dataset contains samples collected from 1995 to 1999.
9. The "2010" contaminant mapping dataset contains samples collected from 2005 to 2013.

**Table 2**
**Equations to Compute Concentrations of Additional Contaminants Using the Proposed Model COPCs**

| Contaminant of Interest | Sediment Concentration | Water Column Concentration |
|---|---|---|
| Total PCBs[1] | 3.0 x Tetra-CB | 3.2 x Tetra-CB |
| PCB-105[2] | 11.0 x PCB-167 | 9.2 x PCB-167 |
| PCB-118[2] | 24.4 x PCB-167 | 22.9 x PCB-167 |
| PCDD/PCDF TEQ (Mammal)[3] | 1.0 x TEQ computed by 2378-TCDD, 12378-PeCDD, 23478-PeCDF, and 1234678-HpCDF | 1.1 x TEQ computed by 2378-TCDD, 12378-PeCDD, 23478-PeCDF, and 1234678-HpCDF |
| PCB TEQ (Mammal)[3] | 1.1 x TEQ computed by PCB-126, PCB-167, PCB-105, and PCB-118 | 1.2 x TEQ computed by PCB-126, PCB-167, PCB-105, and PCB-118 |
| Total TEQ (Mammal)[3] | 1.0 x TEQ computed by 2378-TCDD, 12378-PeCDD, 23478-PeCDF, 1234678-HpCDF, PCB-126, PCB-167, PCB-105, and PCB-118 | 1.1 x TEQ computed by 2378-TCDD, 12378-PeCDD, 23478-PeCDF, 1234678-HpCDF, PCB-126, PCB-167, PCB-105, and PCB-118 |

Notes:

1. See regressions in Figure 1.
2. See regressions in Figure 2.
3. See regressions in Figure 3.

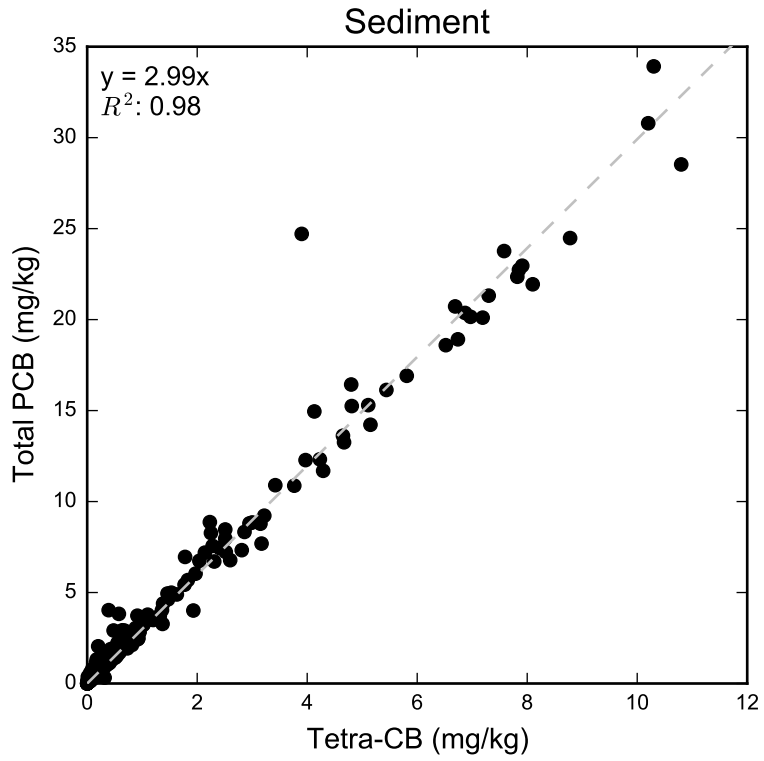
PCB = polychlorinated biphenyl

PCDD = polychlorinated dibenzo-p-dioxin

PCDF = polychlorinated dibenzofuran

TEQ = toxic equivalency quotient

# FIGURES



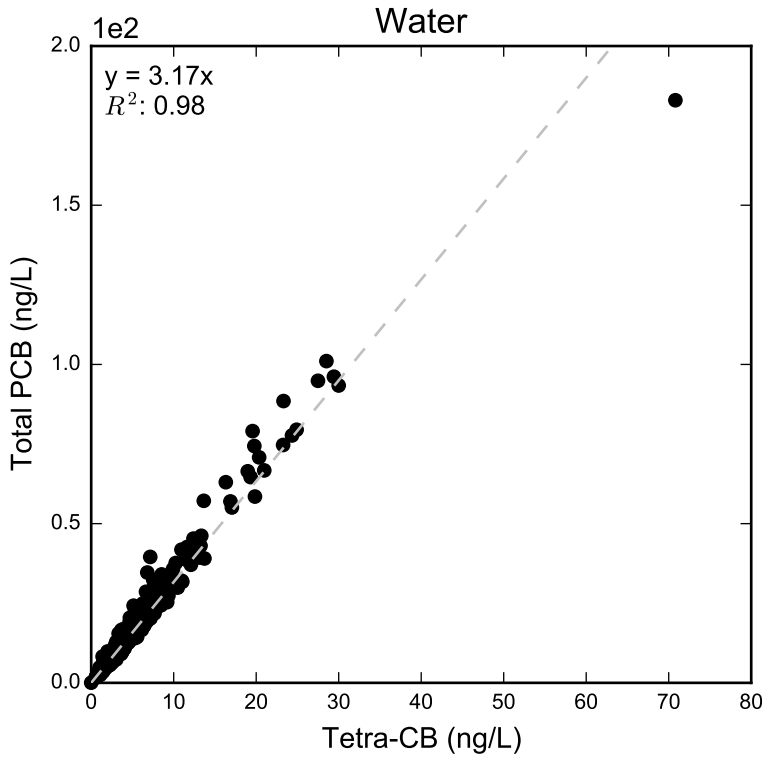




**Figure 1**

Correlations of Total PCB with Tetra-CB in Surface (Top 6 inches) Sediments and Water Column in Lower Passaic River and Newark Bay

*Dashed line represents linear regression without an intercept. Non-detect samples removed.*
*Data sources: Sediment data collected during 2005-2013; water column data collected from sv-CWCM during 2011-2013.*

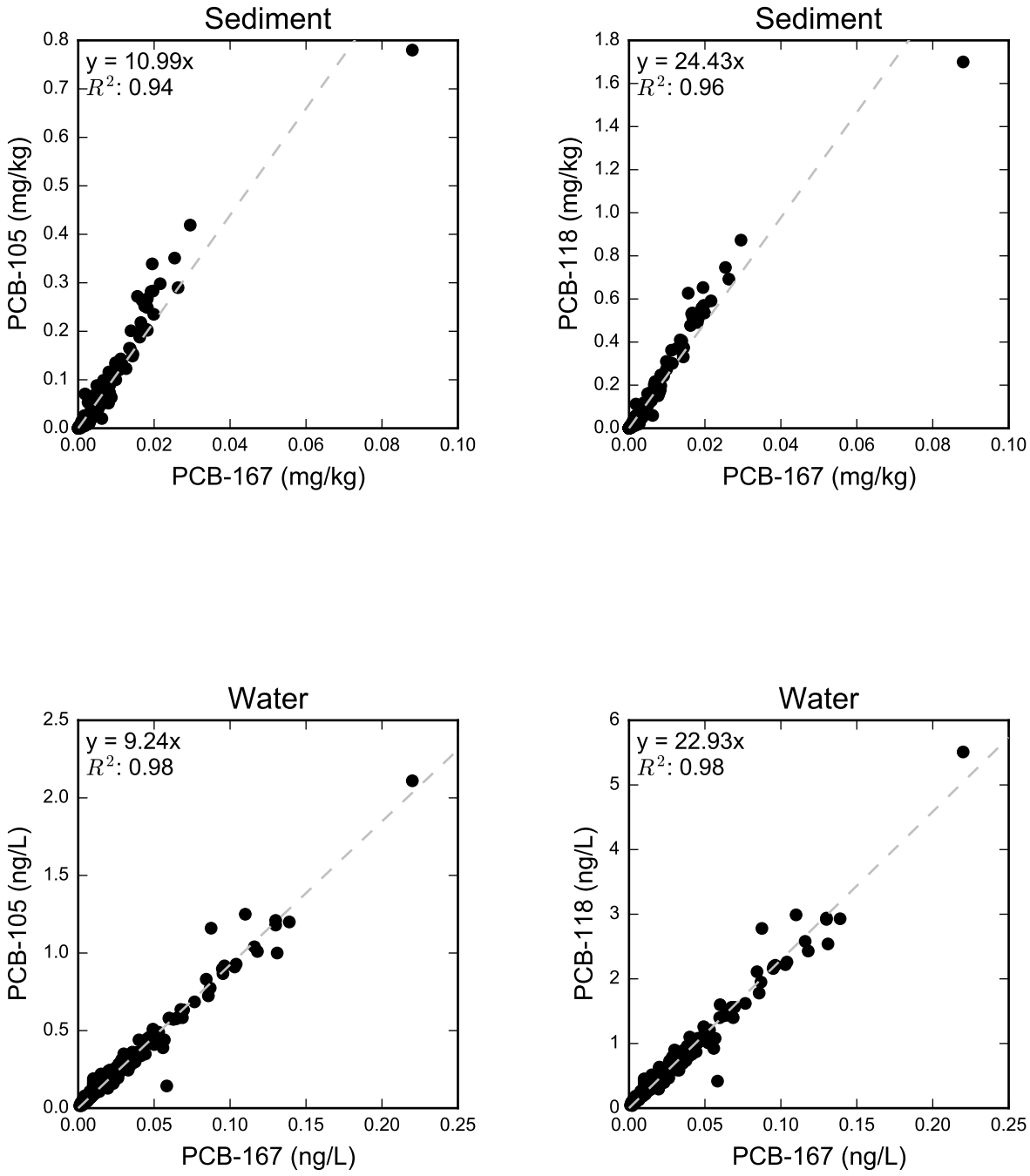
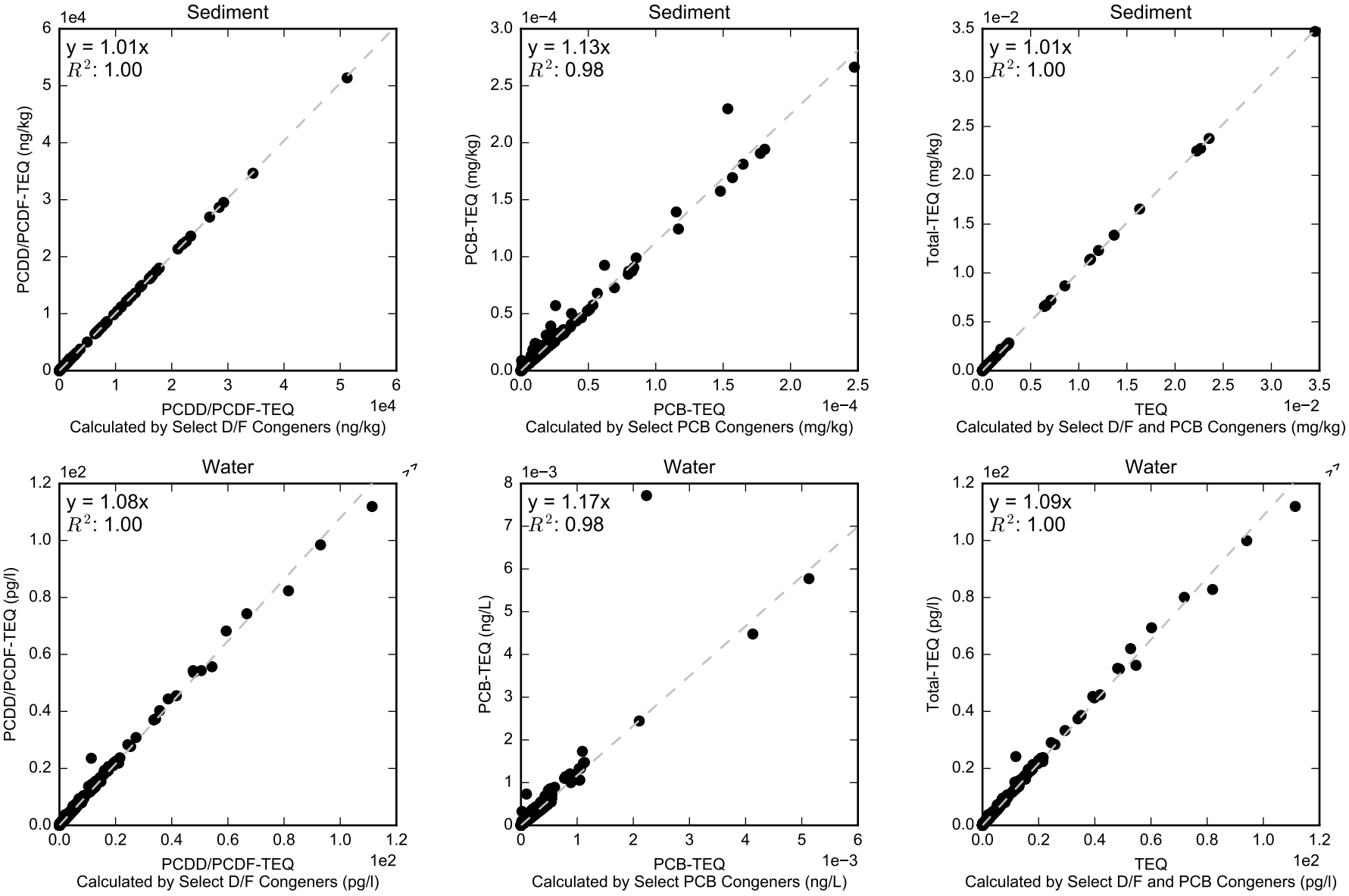



**Figure 2**

Correlations of PCB-105 and PCB-118 with PCB-167 in Surface (Top 6 inches) Sediments and Water Column in Lower Passaic River and Newark Bay

*Dashed line represents linear regression without an intercept. Non-detect samples removed.*
*Data sources: Sediment data collected during 2005-2013; water column data collected from sv-CWCM during 2011-2013.*




| Select D/F Congeners | Select PCB Congeners | Select D/F and PCB Congeners |
|---|---|---|
| 2,3,7,8-TCDD | PCB-167 | 2,3,7,8-TCDD |
| 1,2,3,7,8-PeCDD | PCB-126 | 1,2,3,7,8-PeCDD |
| 2,3,4,7,8-PeCDF | PCB-105 | 2,3,4,7,8-PeCDF |
| 1,2,3,4,6,7,8-HpCDF | PCB-118 | 1,2,3,4,6,7,8-HpCDF |
| | | PCB-167 |
| | | PCB-126 |
| | | PCB-105 |
| | | PCB-118 |

**Figure 3**

Correlations of PCDD/PCDF-TEQ, PCB-TEQ, and total-TEQ with those Calculated by Select PCDD/PCDFs and PCB Congeners in Surface (Top 6 inches) Sediments and Water Column in Lower Passaic River and Newark Bay

*Dashed line represents linear regression without an intercept. Non-detect samples removed.*
*Data sources: Sediment data collected during 2005-2013; water column data collected from sv-CWCM during 2011-2013.*
*For the water column PCB-TEQ regression, one high TEQ sample (0.0077 ng/L) was removed from the regression.*
*For the water column PCDD/PCDF-TEQ and total-TEQ regressions, two high TEQ samples were removed (11A-CE04-TTR1-A & 12F-CE04-TTR1-B).*